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All *trans*-polyacetylene is considered the prototypical broad band gap quasi one-dimensional organic semiconductor. Intrinsic soliton defects have long been known to be crucial to the understanding the observed optical, infrared, and magnetic properties of this system at low doping levels. Magnetic resonance techniques provide powerful experimental probes into the nature and environment of these neutral-radical defects. Despite the importance of the measured hyperfine tensors in the further characterization of these defect centers very few theoretical studies have attempted to calculate these interactions directly. In an earlier work we showed that first-principles spin-polarized local density functional methods reliably predict proton Fermi-contact coupling constants for planar, neutral, organic π-radicals. We have also used these methods to calculate the hyperfine interactions associated with the soliton defect in polyacetylene. Here we compare the results of these soliton studies to very recent experimental results. Our predicted ratio of the negative to positive spin densities is in good agreement with the results of Mehring *et al.*[1] obtained from triple resonance studies. The negative spin densities arise from spin-polarization effects which also cause the soliton level at mid-gap to be split by several tenths of an eV.

[1] M. Mehring *et al*, Snyth. Metals **28**: D399 (1989).

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FIRST PRINCIPLES STUDY OF SOLITON HYPERFINE INTERACTIONS IN POLYACETYLENE*

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[1] M. Mehring *et al.*, Synth. Metals 28: D399 (1989).

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